

Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs

Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species M. Forés, M. Duran and M. Solà	1
Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips	21
Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state U. Lommatzsch and B. Brutschy	35
Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the $SiO^+$ cation including the effect of core correlation Z.-L. Cai and J.P. François	59
An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds A. Dransfeld and D.B. Chesnut	69
Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H C.W. Bauschlicher, Jr. and S.R. Langhoff	79
Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution C.W. Bauschlicher, Jr.	87
Valence photoionization of $C_6H_6$ by the B-spline one-centre expansion density functional method M. Venuti, M. Stener and P. Decleva	95
Solvent effects on NMR spectrum of acetylene calculated by ab initio methods M. Pecul and J. Sadlej	111
The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions O.B. Jenkins and A.B. Doktorov	121
Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff	153
Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings V.A. Benderskii and E.V. Vetoshkin	173

(continued on inside back page)



**ContentsDirect**, the *free* e-mail alerting service, delivers the table of contents for this journal directly to your PC, prior to publication. The quickest way to register for **ContentsDirect** is via the Internet at: <http://www.elsevier.nl/locate/ContentsDirect>. If you don't have access to the Internet you can register for this service by sending an e-mail message to [cdsubs@elsevier.co.uk](mailto:cdsubs@elsevier.co.uk) - specifying the title of the publication you wish to register for.



Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs

Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species M. Forés, M. Duran and M. Solà	1
Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips	21
Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state U. Lommatzsch and B. Brutschy	35
Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the $SiO^+$ cation including the effect of core correlation Z.-L. Cai and J.P. François	59
An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds A. Dransfeld and D.B. Chesnut	69
Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H C.W. Bauschlicher, Jr. and S.R. Langhoff	79
Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution C.W. Bauschlicher, Jr.	87
Valence photoionization of $C_6H_6$ by the B-spline one-centre expansion density functional method M. Venuti, M. Stener and P. Decleva	95
Solvent effects on NMR spectrum of acetylene calculated by ab initio methods M. Pecul and J. Sadlej	111
The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions O.B. Jenkins and A.B. Doktorov	121
Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff	153
Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings V.A. Benderskii and E.V. Vetoshkin	173

(continued on inside back page)



**ContentsDirect**, the *free* e-mail alerting service, delivers the table of contents for this journal directly to your PC, prior to publication. The quickest way to register for **ContentsDirect** is via the Internet at: <http://www.elsevier.nl/locate/ContentsDirect>. If you don't have access to the Internet you can register for this service by sending an e-mail message to [cdsubs@elsevier.co.uk](mailto:cdsubs@elsevier.co.uk) - specifying the title of the publication you wish to register for.



0301-0104(19980815)234:1-3;1-S

## Contents

(continued from page 4 of cover)

REMPI spectroscopy of internal state populations in HBr + Ar free jets: Rotational relaxation of HBr A.E. Belikov, M.M. Ahern and M.A. Smith	195
The librational and vibrational spectra of water in natrolite, $\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10} \cdot 2\text{H}_2\text{O}$ compared with ab-initio calculations C.M.B. Line and G.J. Kearley	207
$^{17}\text{O}$ nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid J. Seliger and V. Žagar	223
Kinetics of the $\text{CN} + \text{CH}_2\text{CO}$ and $\text{NCO} + \text{CH}_2\text{CO}$ reactions M.A. Edwards and J.F. Hershberger	231
Light induced <i>cis-trans</i> isomerization of azo compounds in polymethyl methacrylate S.Yu. Grebenkin and B.V. Bol'shakov	239
Investigation of the $\text{CS}_2^{2+}$ dication using threshold photoelectrons coincidence spectroscopy M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie	249
Fragment ion yields from $\text{CFCl}_3$ photoexcited in regions of the $\text{Cl}2\text{p}$ , the $\text{C}1\text{s}$ , and the $\text{F}1\text{s}$ electron transitions I.H. Suzuki and N. Saito	255
Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda	265
Hole trapping in tri- <i>p</i> -tolylamine-doped poly(styrene) P.M. Borsenberger, W.T. Gruenbaum, U. Wolf and H. Bässler	277
Low-temperature thermoluminescence in poly(methyl-phenylsilylene) A. Kadashchuk, N. Ostapenko, V. Zaika and S. Nešpùrek	285
Effect of $\text{Al}(\text{CO})_x$ complexation on the aluminum oxidation process M.J. McQuaid and J.L. Gole	297
Author index	311
Subject index	315
Instructions to authors	323